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The cornucopia of meaningful leads: Applying deep adversarial autoencoders for new molecule development in oncology

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Abstract

Recent advances in deep learning and specifically in generative adversarial networks have demonstrated surprising results in generating new images and videos upon request even using natural language as input. In this paper we present the first application of generative adversarial autoencoders (AAE) for generating novel molecular fingerprints with a defined set of parameters. We developed a 7-layer AAE architecture with the latent middle layer serving as a discriminator. As an input and output the AAE uses a vector of binary fingerprints and concentration of the molecule. In the latent layer we also introduced a neuron responsible for growth inhibition percentage, which when negative indicates the reduction in the number of tumor cells after the treatment. To train the AAE we used the NCI-60 cell line assay data for 6252 compounds profiled on MCF-7 cell line. The output of the AAE was used to screen 72 million compounds in PubChem and select candidate molecules with potential anticancer properties. This approach is a proof of concept of an artificially-intelligent drug discovery engine, where AAEs are used to generate new molecular fingerprints with the desired molecular properties.

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Keywords

Adversarial autoencoder, Artificial intelligence, Deep learning, Drug discovery, Generative adversarian networks

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